Schwinger-Boson Mean-Field Theory of Mixed-Spin Antiferromagnet L_2BaNiO_5

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Abstract

The Schwinger-boson mean-field theory is used to study the three-dimensional antiferromagnetic ordering and excitations in compounds L_2BaNiO_5, a large family of quasi-one-dimensional mixed-spin antiferromagnet. To investigate magnetic properties of these compounds, we introduce a three-dimensional mixed-spin antiferromagnetic Heisenberg model based on experimental results for the crystal structure of L_2BaNiO_5. This model can explain the experimental discovery of coexistence of Haldane gap and antiferromagnetic long-range order below Néel temperature. Properties such as the low-lying excitations, magnetizations of Ni and rare-earth ions, Néel temperatures of different compounds, and the behavior of Haldane gap below the Néel temperature are investigated within this model, and the results are in good agreement with neutron scattering experiments.

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I. INTRODUCTION

The existence of Haldane gap [1] in the magnetic excitation spectrum has kept the integer-spin one-dimensional (1D) Heisenberg antiferromagnet to be one of the most interesting subjects in condensed matter physics during the past twenty years. The integer-spin Heisenberg antiferromagnetic (AF) chain should have a singlet ground state, exponentially decaying correlations, and a quantum gap, which have been confirmed by numerous theoretical [2,3,4,5,6] and experimental [7,8,9,10] studies. Kennedy and Tasaki have proved that the appearance of Haldane gap in the spin-1 AF chain corresponds to the breaking of a hidden $Z_2 \times Z_2$ symmetry [11]. The recent discovery of coexistence of Haldane gap and AF long-range order (AF LRO) in rare-earth compounds L_2BaNiO_5 with L=$Y, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er$, and Tm [10,12,13,14,15,16] has offered an opportunity to investigate the effect of staggered field on the Haldane chain. The polarized and unpolarized inelastic neutron scattering experiments on L_2BaNiO_5 [14,16] present that, on the one hand, there are AF interactions between spins of rare-earth and Ni ions, which lead to the three-dimensional (3D) AF LRO with Néel temperature (T_N) ranging from $20 - 70K$ [12,13]. On the other hand, these compounds are also characterized by the presence of NiO_6 octahedron chains along a-axis. As is anticipated, above the Néel temperature, energy gap has been found in the excitation propagating along Ni-chain. Also the Haldane gap is discovered to persist in the 3D AF phase and increase with decreasing temperature below T_N [14,15,16].

Recently several theoretical works have focused on the quasi-1D Haldane system L_2BaNiO_5 [17,18,19]. To describe the coexistence of Haldane gap and AF LRO, the nonlinear sigma model in a static staggered magnetic field has been introduced by Maslov and Zheludev [17]. This system has been studied numerically within the density matrix renormalization group method by adopting the model of an 1D spin-1 Heisenberg chain in a static field [18]. In the above studies, the reason for introducing the static staggered field is based on the assumption that there are 3D directly AF exchange interactions between the spins of rare-earth ions, which lead to the AF LRO below T_N. However, it has been pointed out

by some experiments [12,13,14] that spins of Ni ions also play an important role in forming AF LRO, and the two-dimensional mixed-spin Heisenberg model with $s_1 = 1$ and $s_2 = 1/2$ chains staked alternatively has also been adopted for this system [19].

Depending on the experimental finding of crystal structure, we introduce a more suitable 3D mixed-spin AF Heisenberg model to describe the magnetic properties of compounds L_2BaNiO_5. In this model we define $s_1 = 1$ for the spins of Ni ions, and investigate different members of this family by changing the spin value s_2 of rare-earth ions correspondingly. We use the Schwinger-boson mean-field (SBMF) [20,21,22] theory to study this 3D mixed-spin model. The SBMF theory has been successful to the study of spin-integer Heisenberg chains [20,21], and has also been extended to cases with magnetic ordering by identifying the magnetization with the Bose condensation of the Schwinger bosons [20,21,22]. Within this model, we could explain the experimental discovery of coexistence of Haldane gap and AF LRO. The interactions between spins of Ni and rare-earth ions are proved to be very important in forming the AF LRO. Properties such as the magnetization, Haldane gap and Néel temperatures are also discussed for cases with different s_2. Comparing our results with neutron scattering experiments, we find that our findings could explain some experimental discoveries.

The paper is organized as follows: In Sec. II we introduce the 3D mixed-spin Heisenberg model and Schwinger-boson mean-field theory. Our results of the magnetic properties of L_2BaNiO_5 compounds are presented in Sec. III. Finally, we conclude our findings in Sec. IV.

II. MIXED-SPIN HEISENBERG MODEL AND SCHWINGER-BOSON MEAN-FIELD THEORY

The crystal structures of L_2BaNiO_5 compounds have been investigated extensively by neutron scattering experiments [12,13,14]. They belong to the orthorhombic system, having approximate cell Parameters around $a = 3.8\mathring{A}$, $b = 5.8\mathring{A}$ and $c = 11.3\mathring{A}$. In all members

of this compounds, as figure 1(b) shown, strings of distorted NiO_6 octahedron share apical oxygen and form Haldane chains along the a-axis. The intrachain Ni-O-Ni AF superexchange coupling is about 200-300K [12,13,14], which is the strongest magnetic interaction in the compound. While in the bc plane, as figure 1(a) shown, there is one oxygen between the Ni and rare-earth (L)ions, and thus the Ni-O-L interactions establish links between individual Ni chains. This coupling is of the order of tens of Kelvin (10-30K). Figure 1(a) also shows that there are L-O-L AF interactions between rare-earth ions, which is of the order of 1K or less.

Based on the experimental discovery of the crystal structure of compounds L_2BaNiO_5, we introduce a 3D mixed-spin AF Heisenberg model expressed by the Hamiltonian

$$H = J_1 \sum_{i,\eta_a} S_{1,i} \cdot S_{1,i+\eta_a} + J_2 \sum_{i,\eta_b,\eta_c} S_{1,i} \cdot S_{2,i+\eta_b+\eta_c} + J_3 \sum_{j} S_{2,j} \cdot S_{2,j+\widehat{c_0}} \ , \tag{1}$$

where S_1 and S_2 are the spin operators of Ni and rare-earth ions respectively. η_b and η_c denote a sum over nearest-neighbor (NN) bonds in the bc plane, and so is η_a for the NN bonds along the a-axis. The AF superexchange couplings along the Ni chain, between L and Ni ions, and among the rare-earth L ions are represented as J_1, J_2, and J_3 respectively as figure 1(a) shown.

The Schwinger-boson theory introduces $S_i = \frac{1}{2} b^+_{i\alpha} \sigma_{\alpha,\beta} b_{i\beta}$ (α (or β)=$\uparrow, \downarrow$) [20,21], and the spin degrees of freedom are mapped to the boson degrees of freedom. Meanwhile the original spin Hilbert space corresponds to a boson Hilbert subspace in which $b^+_{i\uparrow} b_{i\uparrow} + b^+_{i\downarrow} b_{i\downarrow} = 2s_i$. These constraints to the boson Hilbert space are imposed in the Hamiltonian (1) by introducing two kinds of Lagrangian multipliers $\lambda_1(i)$ and $\lambda_2(j)$. In addition, we define the bond operators as $Q_a(i,\eta_a) = b_{1i\uparrow} b_{1(i+\eta_a)\downarrow} - b_{1i\downarrow} b_{1(i+\eta_a)\uparrow}$, $Q_h(i,\eta_b,\eta_c) = b_{1i\uparrow} b_{2(i+\eta_b+\eta_c)\downarrow} - b_{1i\downarrow} b_{2(i+\eta_b+\eta_c)\uparrow}$, and $Q_c(j,\widehat{c_0}) = b_{2j\uparrow} b_{2(j+\widehat{c_0})\downarrow} - b_{2j\downarrow} b_{2(j+\widehat{c_0})\uparrow}$. The Hamiltonian (1) can be rewritten as

$$\begin{aligned} H = & -\frac{1}{2} J_1 \sum_{i,\eta_a} \left\{ Q^+_a(i,\eta_a) Q_a(i,\eta_a) - 2s_1^2 \right\} - \frac{1}{2} J_3 \sum_j \left\{ Q^+_c(j,\widehat{c_0}) Q_c(j,\widehat{c_0}) - 2s_2^2 \right\} \\ & -\frac{1}{2} J_2 \sum_{i,\eta_b,\eta_c} \left\{ Q^+_h(i,\eta_b,\eta_c) Q_h(i,\eta_b,\eta_c) - 2s_1 s_2 \right\} \\ & + \sum_i \lambda_1(i) \left\{ b^+_{1i\uparrow} b_{1i\uparrow} + b^+_{1i\downarrow} b_{1i\downarrow} - 2s_1 \right\} + \sum_j \lambda_2(j) \left\{ b^+_{2j\uparrow} b_{2j\uparrow} + b^+_{2j\downarrow} b_{2j\downarrow} - 2s_2 \right\} . \end{aligned} \tag{2}$$

Next, we make a Hartree-Fock decomposition of Eq. (2) by taking the average values of the bond operators and Lagrange multipliers to be uniform and static as $\langle Q_a(i,\eta_a)\rangle = Q_a$, $\langle Q_h(i,\eta_b,\eta_c)\rangle = Q_h$, $\langle Q_c(j,\widehat{c_0})\rangle = Q_c$, $\langle \lambda_1(i)\rangle = \lambda_1$, and $\langle \lambda_2(j)\rangle = \lambda_2$. Under the Fourier transformation, we obtain the following mean-field Hamiltonian in the momentum space

$$\begin{aligned} H^{MF} = & \sum_k 2Z_k \left\{ b_{1k\uparrow} b_{1(-k)\downarrow} - b_{1k\downarrow} b_{1(-k)\uparrow} + h.c \right\} + \sum_k 4D_k \left\{ b_{1k\uparrow} b_{2(-k)\downarrow} - b_{1k\downarrow} b_{2(-k)\uparrow} + h.c \right\} \\ & + \sum_k 2\chi_k \left\{ b_{2k\uparrow} b_{2(-k)\downarrow} - b_{2k\downarrow} b_{2(-k)\uparrow} + h.c \right\} + \sum_{k\sigma} \left\{ 4\lambda_1 b^+_{1k\sigma} b_{1k\sigma} + 8\lambda_2 b^+_{2k\sigma} b_{2k\sigma} \right\} \\ & + 2N \left\{ J_1 Q_a^2 + 4J_2 Q_h^2 + J_3 Q_c^2 - 4\lambda_1 s_1 + 2J_1 s_1^2 + 8J_2 s_1 s_2 + 2J_3 s_2^2 - 8\lambda_2 s_2 \right\}, \end{aligned} \tag{3}$$

where $Z_k = J_1 Q_a \cos(k_z a_0)$, $\chi_k = J_3 Q_c \cos(k_x c_0)$, and $D_k = 2J_2 Q_h \cos(k_x c_0)\cos(k_y b_0)$.

Diagonalizing H^{MF} in Eq. (3) by the Bogoliubov transformation, we obtain

$$H^{MF} = 2\sum_k \left\{ E_k^+ \left(\alpha^+_{1k\sigma}\alpha_{1k\sigma} + \alpha_{2k\sigma}\alpha^+_{2k\sigma} \right) + E_k^- \left(\beta^+_{1k\sigma}\beta_{1k\sigma} + \beta_{2k\sigma}\beta^+_{2k\sigma} \right) \right\} + E_0 \tag{4}$$

with

$$\begin{aligned} E_k^{\pm} &= \sqrt{\frac{A \pm \sqrt{A^2 - 4B}}{2}} \\ A &= \lambda_1^2 + 4\lambda_2^2 - \left(Z_k^2 + \chi_k^2 + 2D_k^2 \right) \\ B &= 4\lambda_1\lambda_2 \left(\lambda_1\lambda_2 - D_k^2 \right) - \chi_k^2\lambda_1^2 - 4Z_k^2\lambda_2^2 + \left(\chi_k Z_k - D_k^2 \right)^2 \\ E_0 &= 2N \left\{ J_1 Q_a^2 + 4J_2 Q_h^2 + J_3 Q_c^2 + 2J_1 s_1^2 + 8J_2 s_1 s_2 + 2J_3 s_2^2 \right\} \\ & \quad -8N\lambda_1 \left(s_1 + \frac{1}{2} \right) - 16N\lambda_2 \left(s_2 + \frac{1}{2} \right). \end{aligned} \tag{5}$$

Furthermore, the mean-field free energy is given by

$$F^{MF} = \frac{8}{\beta} \sum_k \ln \left\{ \left(2\sinh \left(\frac{\beta E_k^+}{2} \right) \right) + \ln \left(2\sinh \left(\frac{\beta E_k^-}{2} \right) \right) \right\} + E_0. \tag{6}$$

The mean-field equations are obtained by differentiating F^{MF} with respect to the parameters Q_a, Q_h, Q_c, λ_1, and λ_2 as

$$\frac{\partial F^{MF}}{\partial Q_a} = \frac{\partial F^{MF}}{\partial Q_h} = \frac{\partial F^{MF}}{\partial Q_c} = \frac{\partial F^{MF}}{\partial \lambda_1} = \frac{\partial F^{MF}}{\partial \lambda_2} = 0. \tag{7}$$

Thus we obtain five self-consistent equations to determine the average values of the bond operators and Lagrange multipliers.

III. MEAN-FIELD SOLUTIONS

In this section, we present the solutions of the SBMF theory. The experimental discovery of coexistence of Haldane gap and AF LRO below T_N are obtained by our study. As equation (5) shown, there are two branches of the magnetic excitations E_k^+ and E_k^-, which have quite different behaviors below T_N. On the one hand, the magnetic excitation E_k^+ has an energy gap in the whole temperature region, and below T_N this energy gap increases with decreasing temperature. On the other hand, within the temperature region from zero to T_N, E_k^- keeps to be gapless and has its minimal value $E_k^- = 0$ at $k = 0$. Under this condition, the Schwinger-boson condensation occurs and leads to the AF LRO in this system. In our calculation, we introduce the Schwinger-boson condensation into the self-consistent mean-field equations, and obtain the temperature dependence of the magnetizations of Ni (M_1) and rare-earth (M_2) ions below T_N respectively. The magnetizations M_1 and M_2 are expressed as

$$M_1 = \langle S_1^Z \rangle = \frac{1}{2N} \sum_i \langle b_{1i\uparrow}^+ b_{1i\uparrow} - b_{1i\downarrow}^+ b_{1i\downarrow} \rangle$$
$$M_2 = \langle S_2^Z \rangle = \frac{1}{2N} \sum_j \langle b_{2j\uparrow}^+ b_{2j\uparrow} - b_{2j\downarrow}^+ b_{2j\downarrow} \rangle. \quad (8)$$

We choose the AF superexchange interactions as $J_1 = J$, $J_2 = 0.1J$ and $J_3 = 0.01J$ ($J > 0$) according to the experimental studies of the magnetic properties of compounds L_2BaNiO_5 [12,13,14]. The AF interactions between Ni ions has been estimated as $2J = 200 - 300K$ by the neutron scattering experiments [12,14]. To make it simple and clear, in our calculation we choose $J = 100K$.

The neutron scattering experimental results of Nd_2BaNiO_5 obtained by Yokoo *et al.* [15] are shown in Fig. 2(a) and 2(b) (open circles). The solid lines in Fig. 2(a) and 2(b) show fits to the above experimental results by our numerical calculations for the case with $s_2 = 3/2$ respectively. The temperature dependence of magnetizations M_1/s_1 and M_2/s_2 for the cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$, and 3 are shown in figure 2(c) and 2(d) respectively. As temperature increases, the thermal fluctuation in the system becomes stronger, and the magnetizations decrease rapidly and drop to zero at the Néel temperatures. Therefore, we

could also determine the Néel temperatures T_N for all members of the L_2BaNiO_5 family through our calculation.

In figure 3, we plot the Néel temperature T_N as a function of spin value s_2 (filled circles and dotted line). For comparison, the Néel temperatures of compounds Ho_2BaNiO_5 ($T_N = 53K$) [12], Nd_2BaNiO_5 ($T_N = 48K$) [13] and Pr_2BaNiO_5 ($T_N = 24K$) [14] obtained by the neutron scattering experiments are also shown in Fig. 3 (filled triangles). Our theoretical results roughly agree with the experimental results. We also obtain that the Néel temperature T_N increases monotonously with the increasing of s_2. As the spin value of the rare-earth ions s_2 equal to $1/2$ and 3, we get that the minimize and maximum Néel temperature are $T_N^{Min} \approx 0.207J$ and $T_N^{Max} \approx 0.872J$ respectively. Our result of the Néel temperature region is approximately from $20.7K$ to $87.2K$ when $J = 100K$, which is in good agreement with the experimental estimation of T_N region $20 - 70K$ [12,13].

The two branches of the magnetic excitation E_k^+ and E_k^- represent the spin fluctuations along the a-axis and within bc plane respectively. In the exactly one-dimensional case ($J_2 = J_3 = 0$), the excitation E_k^- vanishes and the energy gap of E_k^+ is just the Haldane gap of AF Heisenberg chain, which is closely related to the breaking of a hidden $Z_2 \times Z_2$ symmetry [11]. We obtain that the coexistence of Haldane gap and AF LRO below T_N is a common feather of all members of compounds L_2BaNiO_5 except Y_2BaNiO_5. The neutron scattering experiments have discovered that, below the Néel temperature, the Haldane gap increases as the temperature decreases [14,15,16]. The temperature dependences of the Haldane gap Δ for the cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$ and 3 are also investigated by the SBMF theory and the behaviors are shown in figure 4(a) respectively. The temperature dependence of the energy gap Δ obtained by our calculation is found to agrees with the experimental discovery.

Our calculation also implies that the effect of the staggered magnetization on the magnetic excitation is to widen the Haldane gap. Below T_N, the effective internal magnetic field H_{eff} imposed on the Haldane chain is assumed approximately as the magnetization M_1 of Ni ions. This field is found to increase with the decreasing of temperature and the increasing of spin value s_2 because of the thermal fluctuation being weakened and the AF

ordering being enhanced. In figure 4(b), we plot the energy gap Δ of zero temperature as a function of H_{eff}, and we find that H_{eff} has strong effect to widen the Haldane gap.

In addition, based on the 3D mixed-spin model, we obtain that AF LRO below the Néel temperature is not constructed only by the rare-earth ions. Our results support the suggestion that Ni ions also play an important role in forming the AF LRO. We plot in figure 5 the Néel temperature as a function of AF coupling J_2 in the cases with $s_2 = 1/2$, $J_1 = J$, and $J_3 = 0.01J$. In compounds L_2BaNiO_5, the effective interactions between individual Ni chains rely on the AF coupling J_2 between Ni^{2+} and rare-earth L^{3+}. We obtain that the Néel temperature rises rapidly with the increase of J_2 as shown in figure 5, so the coupling J_2 are important in forming the AF LRO. Besides, as $J_2 = 0$, there are no interactions between Ni chains and thus the Néel temperature drops to zero. The Haldane excitation energy E_k^+ in 3D and 1D cases are shown in figure 6(a) and 6(b) respectively. Here we choose $s_2 = 1/2$, $J_1 = J$, $J_2 = 0.01J$, $J_3 = 0.01J$, and $k_x = k_y = 0$ for the 3D case, and obtain that the corresponding Néel temperature is $T_N = 0.206J$. To compare the behaviors of magnetic excitations below and above the Néel temperature, we study two conditions of $T = 0.1$ (solid lines) and $T = 0.4J$ (dotted lines) respectively for both 1D and 3D cases. In the 3D case, we find, in figure 6(a), that the energy gap below the Néel temperature is obviously bigger than that above the Néel temperature, which is in opposition with the behavior for pure 1D case (shown in figure 6(b)). In addition, we obtain that the thermal fluctuation has strong effect to destroy the 3D spin correlations in the compounds, as a result the behaviors in 3D case is the same as that in 1D case when temperature is above the Néel temperature.

IV. SUMMARY

In conclusion, we have introduced a 3D mixed-spin AF Heisenberg model based on the experimental results of the crystal magnetic structure of compounds L_2BaNiO_5, and studied this model with the SBMF theory. The experimental discovery of coexistence of Haldane gap and AF LRO below T_N has been deduced by our calculation. Properties such as the low-

lying excitations, magnetizations of Ni and rare-earth ions, Néel temperatures of different members of this family and behavior of Haldane gap below T_N have also been investigated within this model.

We have obtained two branches of the magnetic excitations E_k^+ and E_k^-, of which E_k^+ has an energy gap and E_k^- is gapless below T_N. The theoretical result of the Néel temperature region is approximately from $20.7K$ to $87.2K$, which is in good agreement with the experimental estimation of the region $20 - 70K$. We have also obtained that Haldane gap increases with decreasing temperature, and the effect of the magnetization is to widen the Haldane gap. Our results are in good agreement with the experimental discoveries. Our findings also support the suggestion that the AF LRO below T_N is not constructed only by the rare-earth ions, and Ni ions also play an important role in forming the AF LRO.

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FIGURES

FIG. 1. (a) Structural relation between Ni and rare-earth sites in the bc plane, and (b) Ni and apical oxygen form the Haldane chain along the a-axis.

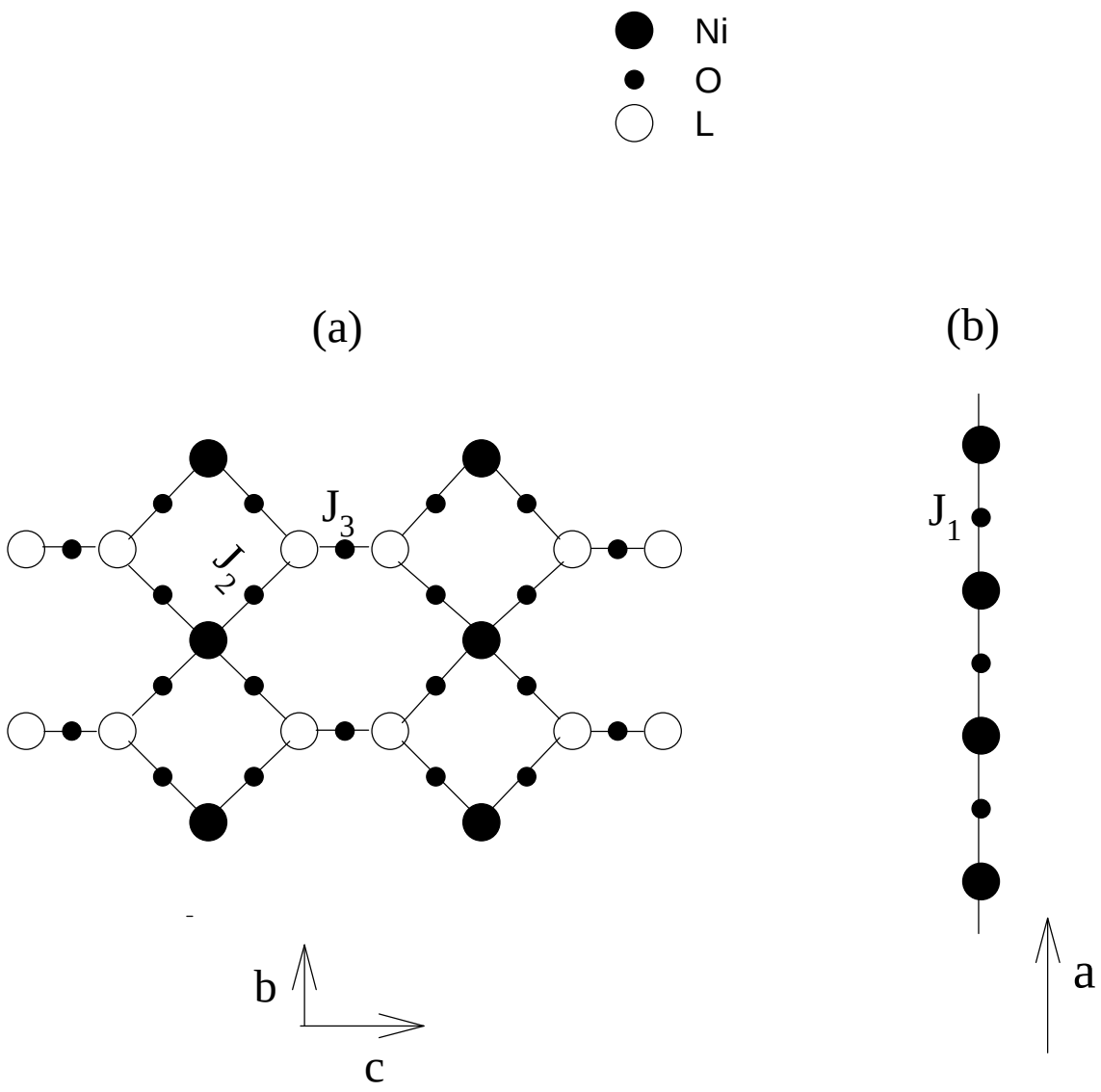
FIG. 2. The temperature dependence of the ordered moment on the Ni (a) and Nd (b) sites in Nd_2BaNiO_5 sample taken from Ref. 14 (open circles), and the solid lines show fits to the experimental discovery by our numerical results of the case with $s = 3/2$ respectively; Magnetizations M_1/s_1 (c) and M_2/s_2 (d) as functions of temperature below T_N for cases of $s_2 = 1/2, 1, 3/2, 2, 5/2,$ and 3 respectively.

FIG. 3. Néel temperatures of the compounds L_2BaNiO_5 for the cases with different spin value s_2. The circles represent the theoretical results, and the triangles are experimental findings of compounds Nd_2BaNiO_5, Pr_2BaNiO_5 and Ho_2BaNiO_5 taken from Ref. 11-13.

FIG. 4. (a) The temperature dependence of Haldane gap for cases of $s_2 = 1/2, 1, 3/2, 2, 5/2$ and 3 below the Néel temperatures respectively; (b) The Haldane gap as a function of the effective internal magnetic field H_{eff}.

FIG. 5. Néel temperature as a function of AF coupling J_2 between Ni^{2+} and L^{3+} ions of case $s_2 = 1/2$, $J_1 = J$, and $J_3 = 0.01J$.

FIG. 6. The branch of Haldane excitation E_k^+ as a function of k_z in (a) 3D with $s_2 = 1/2$, $J_1 = J$, $J_3 = 0.01J$ and (b) pure 1D cases. The solid lines show results of temperature $T = 0.1J$, and the dotted lines present results of $T = 0.4J$.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b
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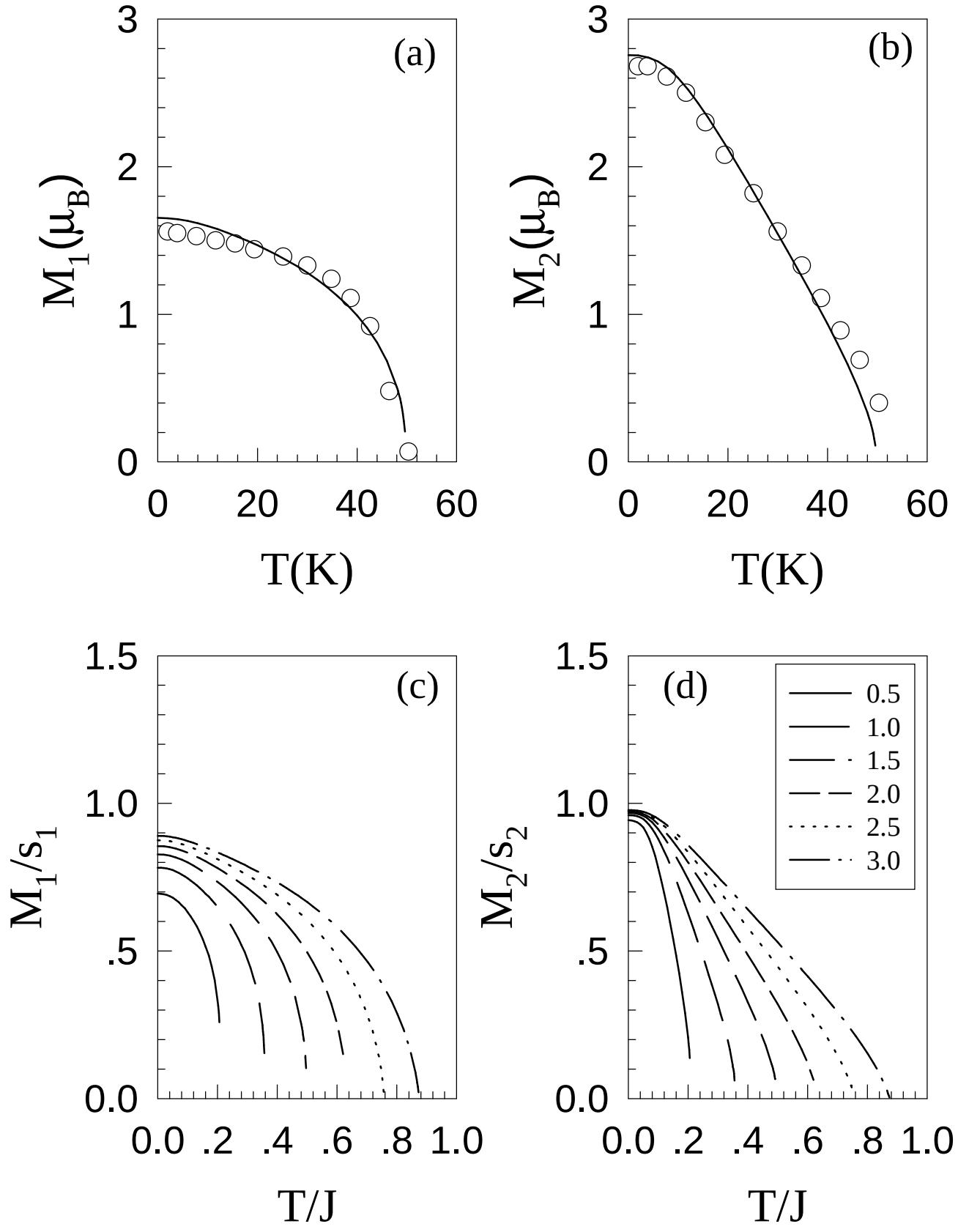
(a)
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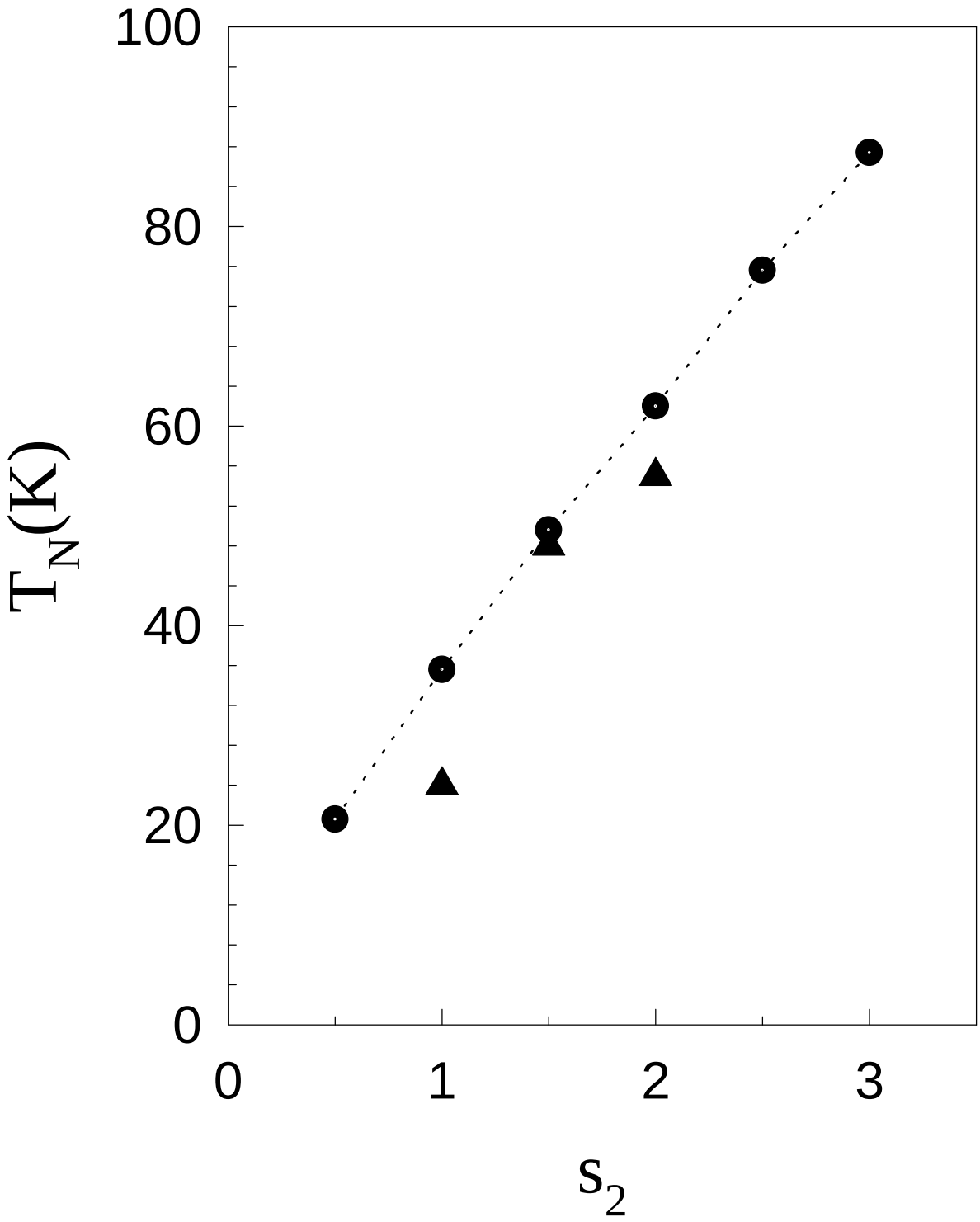
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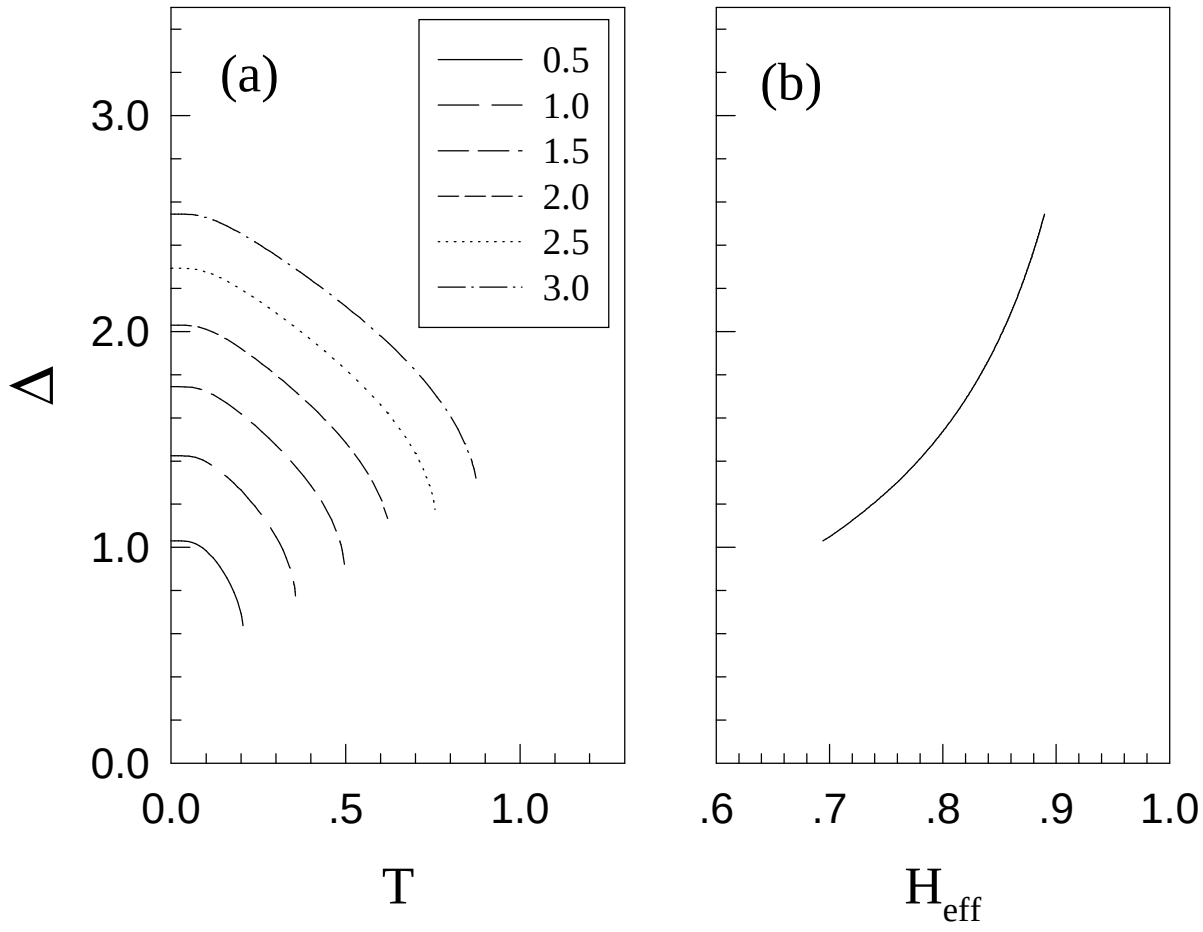
(a)
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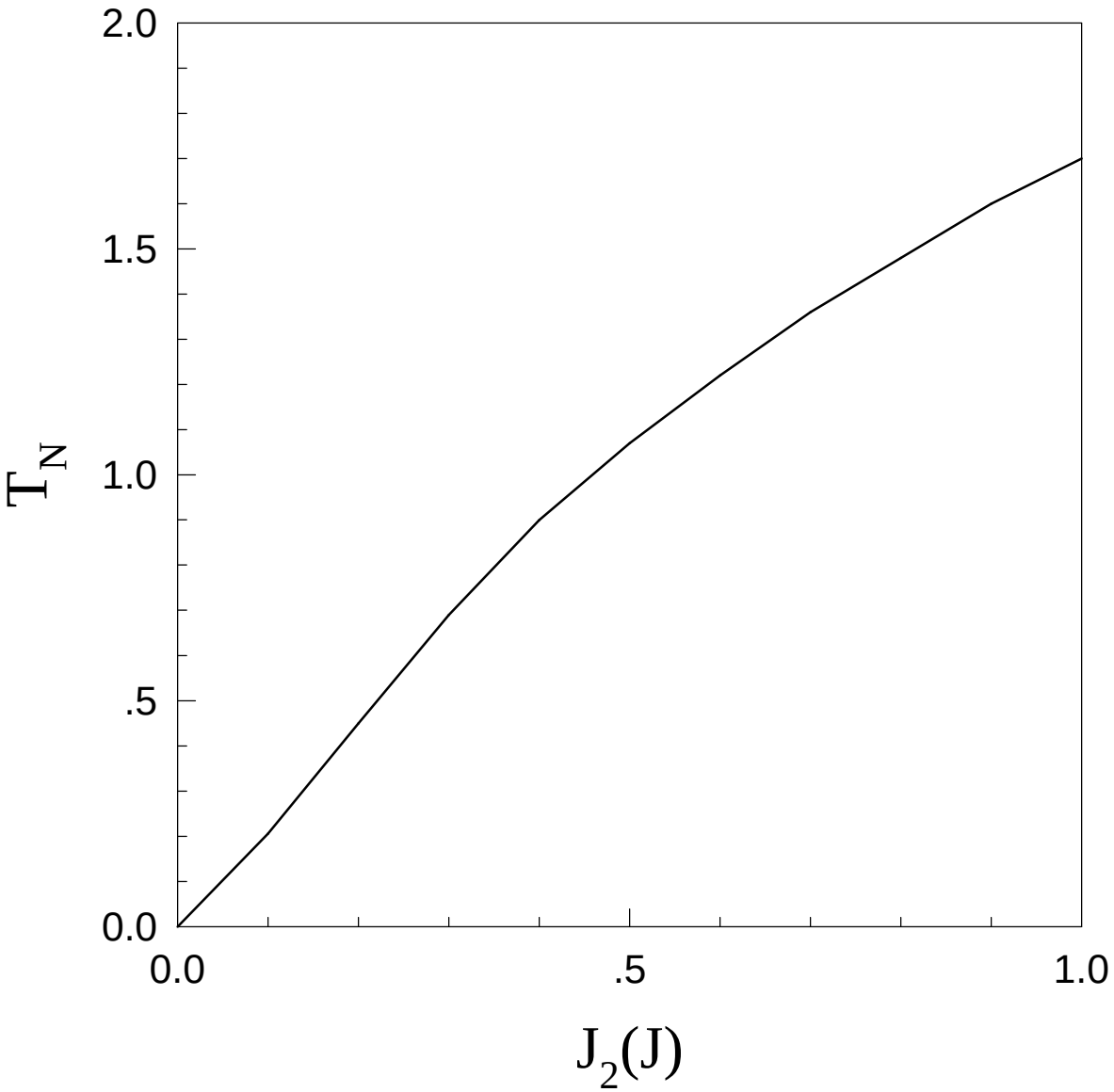
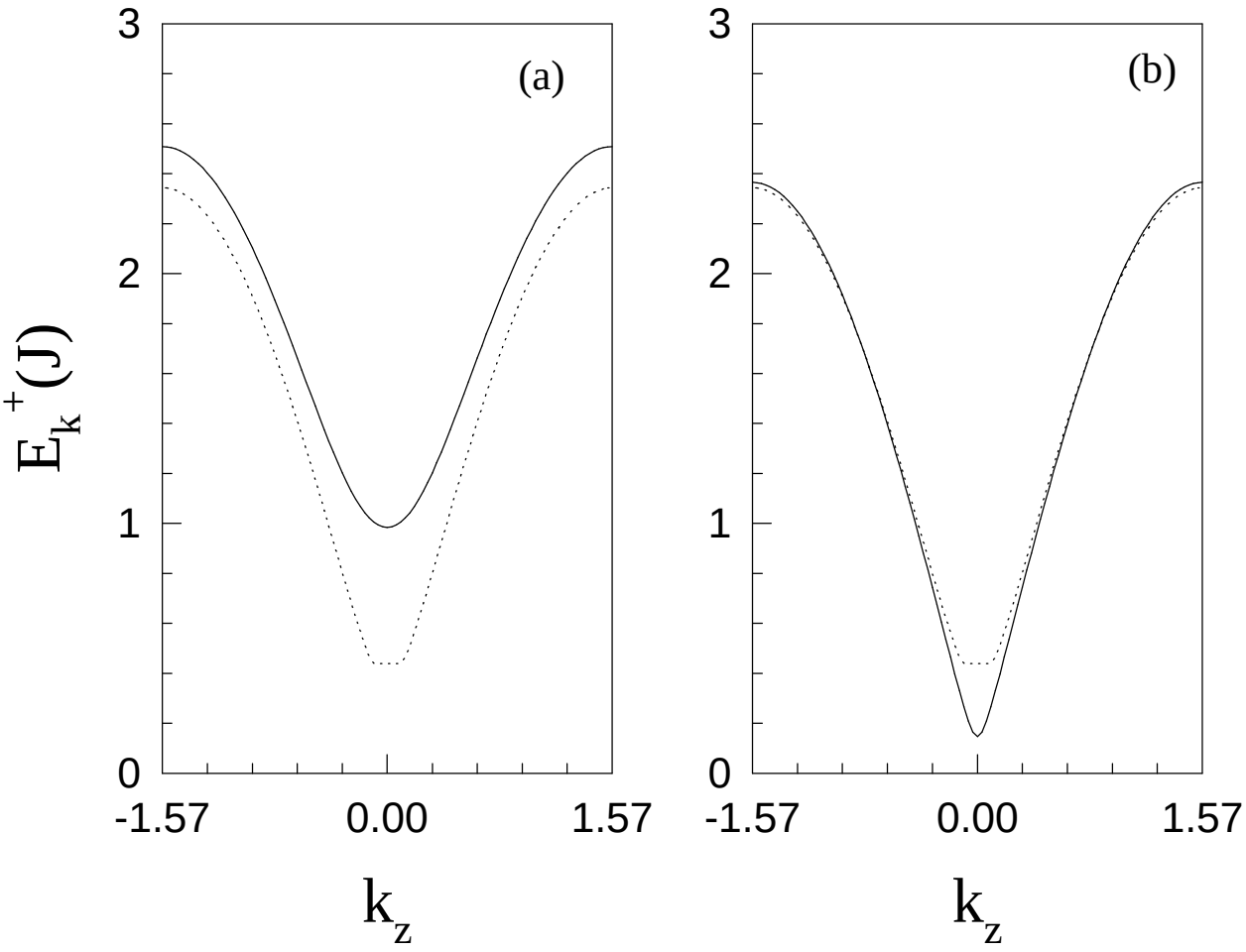
3.0
2.0
1.0
0.0
0.0
.5
1.0
T
.6
.7
.8
.9
1.0
H_eff


2.0
1.5
1.0
.5
0.0
T_N
0.0
.5
1.0
$J_2(J)$


3
2
1
0
(a)
(b)
E_k^+ (J)
-1.57
0.00
1.57
k_z